

SimulationType MonteCarlo
NumberOfCycles 10000
NumberOfInitializationCycles 5000
PrintEvery 500
RestartFile no

ChargeMethod Ewald
CutOff 12.0
Forcefield Dubbeldam2007FlexibleIRMOF-1
EwaldPrecision 1e-6

Framework 0
FrameworkName IRMOF-1
UnitCells 1 1 1
HeliumVoidFraction 0.826
FrameworkDefinitions Dubbeldam2007FlexibleIRMOF-1
ExternalTemperature 298.15
ExternalPressure 1.0e5

Component 0 MoleculeName H2
MoleculeDefinition TraPPE
IdealGasRosenbluthWeight 1.0
TranslationProbability 1.0
RotationProbability 1.0
ReinsertionProbability 1.0
SwapProbability 1.0
CreateNumberOfMolecules 0